

Bose Hubbard model in the presence of Ohmic dissipation

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We study the zero temperature mean-field phase diagram of the Bose-Hubbard model in the presence of local coupling between the bosons and an external bath. We consider a coupling that conserves the on-site occupation number, preserving the robustness of the Mott and superfluid phases. We show that the coupling to the bath renormalizes the chemical potential and the interaction between the bosons and reduces the size of the superfluid regions between the insulating lobes. For strong enough coupling, a finite value of hopping is required to obtain superfluidity around the degeneracy points where Mott phases with different occupation numbers coexist. We discuss the role that such a bath coupling may play in experiments that probe the formation of the insulator-superfluid shell structure in systems of trapped atoms.

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The Bose-Hubbard model (BHM) describes a wide variety of physical situations for appropriate parameter ranges [1]: Josephson junction arrays, ultracold atoms in optical lattices [2, 3], and polaritons or photons in arrays of resonant optical cavities [4, 5]. A key feature of the BHM is the existence of a transition between Mott insulator and superfluid phases, recently observed for cold atoms in optical lattices [6, 7, 8]. This superfluid-insulator transition (SIT) is well understood theoretically [9, 10, 11] and occurs as the magnitude of the inter-site hopping J is varied relative to the on-site repulsion U . At $T = 0$, there are insulating Mott phases for small enough J/U which exist in well-defined domains (Mott lobes) in the zJ/U - μ/U plane (μ is the chemical potential and z is the co-ordination), while in the large J limit there is a superfluid state with fully delocalized particles.

In some, or all, of the various systems that are described by the BHM, it is likely that there will be coupling to external degrees of freedom in the environment that can be modelled as a bath that lead to equilibration in the BH system. At small but finite temperatures, the insulating nature of the Mott phase does not change, although the on-site occupation numbers undergo thermal fluctuations leading to finite compressibility [12]. Experiments on optical lattice systems are in this regime, where temperature is important [13]. However, it is still a matter of debate whether heating takes place as the depth of the lattice potential is increased [14, 15]. It has been suggested that the main cause for such a temperature rise is the increase of the excitation energy gap combined with the necessity of maintaining a constant entropy [13, 16, 17]. If heating can be important, then maintaining the system at a constant temperature may require the presence of some source of dissipation to remove energy. The issue of dissipative dynamics in cold atom systems has attracted considerable recent attention, in the contexts of cooling atoms in the lowest Bloch band [18], Bose-Fermi mixtures [19], the decay of su-

percurrents [20, 21], and one dimensional cold molecular gases [22]. Hence, it is of great interest to address theoretically the issue of how coupling to a heat bath affects the phase diagram of the BHM.

In this Letter we investigate the influence of coupling to a heat bath (assumed to be Ohmic) on the standard phase diagram of the BHM [9, 10, 11]. We assume that the system of bosons is in full equilibrium with the bath at fixed temperature. Throughout our treatment, we assume for simplicity that $T = 0$, but briefly mention possible changes in the phase diagram due to finite temperature. We consider a coupling between the bath and bosons through the particle operator \hat{n}_i , implying that the number of bosons in the system is fixed. Hence the Mott insulator may still be defined as a state with integer expectation value for the occupation number n_0 on each site, and in the superfluid phase there is a finite phase stiffness. The coupling to a bath leads to: i) Renormalization of μ and U to μ' and U' respectively, which determine n_0 in the Mott regions; ii) the regions of superfluidity between the Mott lobes shrink in size on the zJ/U - μ/U phase diagram. If the coupling to the bath is strong enough, superfluidity is absent for small zJ/U regardless of μ , illustrating that coupling to external degrees of freedom inhibits the formation of a phase coherent state. We discuss possible connections of our findings to measurements performed in the presence of a magnetic trap potential and suggest how the coupling to a bath might be detected.

The starting point of our calculations is the standard BH Hamiltonian, and we assume that the bosons couple locally to the heat bath, so that the total Hamiltonian is

$$\hat{H} = \hat{H}_{bos} + \hat{H}_{bath} + \hat{H}_{coup}, \quad (1)$$

where \hat{H}_{coup} describes coupling to the bath. The boson Hamiltonian \hat{H}_{bos} consists of a local piece H_0 and a hop-

ping term H_J :

$$\begin{aligned} \hat{H}_{bos} = & -J \sum_{\langle i,j \rangle} (\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i) - \mu \sum_i \hat{n}_i \\ & + \sum_i \frac{U}{2} \hat{n}_i (\hat{n}_i - 1) = \hat{H}_J + \hat{H}_0, \end{aligned} \quad (2)$$

$$\hat{H}_{bath} = \sum_{i\alpha} \varepsilon_\alpha \hat{b}_{i\alpha}^\dagger \hat{b}_{i\alpha}, \quad (3)$$

$$\hat{H}_{coup} = \sum_{i\alpha} g_\alpha (\hat{b}_{i\alpha}^\dagger + \hat{b}_{i\alpha}) \hat{n}_i. \quad (4)$$

$\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ is the on-site number operator, and the notation $\langle i, j \rangle$ indicates that the summation is restricted to nearest neighbors only. The operators $\hat{b}_{i\alpha}^\dagger$ and $\hat{b}_{i\alpha}$ create and annihilate the bath degrees of freedom which have an energy spectrum ε_α . This form of coupling, in which the bath degrees of freedom are coupled to the on-site density \hat{n}_i , is most suitable to take into account fluctuations of the chemical potential. g_α characterizes the strength of the coupling, which we assume to be purely local and Ohmic:

$$g_\alpha^2 = \eta \varepsilon_\alpha \exp \{-\varepsilon_\alpha / \Lambda\}, \quad (5)$$

where η is the strength of the coupling to the bath, and Λ is the energy cutoff for the bath degrees of freedom. The inverse cutoff $1/\Lambda$ represents the time scale for inertial effects in the bath [23]. We note that the model we consider is similar to that of trapped impurity atoms in a Bose-Einstein condensate considered in Ref. [24].

We focus on the mean-field phase diagram that, in the absence of the bath, can be obtained by decoupling the tunneling term \hat{H}_J and finding self-consistently the condition for a non-zero mean-field superfluid order parameter Ψ_B . Our main goal here is to elucidate the qualitative effects of the coupling to a bath, hence our use of mean field theory – future work will investigate effects beyond mean field theory. Identical results are obtained if one derives the partition function with the effective action that describes fluctuations of Ψ_B close to the transition line in the Mott phase. Following the line of Refs. [10, 25], we write down the effective mean-field Hamiltonian:

$$\hat{H}_{MF} = \hat{H}_0 + \hat{H}_{bath} + \hat{H}_{coup} - \sum_i \left(\Psi_B \hat{a}_i^\dagger + \Psi_B^* \hat{a}_i \right). \quad (6)$$

The optimum value for $\Psi_B = zJ \langle \hat{a}_i \rangle$ and is in fact proportional to the superfluid density, with z being the coordination number. This can be seen, if we add and subtract \hat{H}_{MF} from \hat{H} , so that the mean-field value of the ground state energy per site is [10]

$$\tilde{E}_0 = \tilde{E}_{MF}(\Psi_B) - zJ \langle \hat{a}_i^\dagger \rangle \langle \hat{a}_i \rangle + \langle \hat{a}_i \rangle \Psi_B^* + \langle \hat{a}_i^\dagger \rangle \Psi_B. \quad (7)$$

$\tilde{E}_{MF}(\Psi_B)$ is determined by the occupation number $n_0(\mu/U)$ in the corresponding Mott region, but here it is also a function of the parameters η and Λ characterizing the bath. Since terms involving Ψ_B and Ψ_B^* can be

treated as a perturbation in the Mott-insulator phases, we can expand \tilde{E}_{MF} in powers of Ψ_B and Ψ_B^* [26]

$$\tilde{E}_{MF} = \tilde{E}_{MF}^{(0)} + \chi |\Psi_B|^2 + \mathcal{O}(|\Psi_B|^4). \quad (8)$$

In general χ is a function of all parameters characterizing the local part of the Hamiltonian. Self-consistently minimizing Eqs. (7) and (8), we obtain that Ψ_B has a positive non-zero value once the condition $1/zJ = \chi$ is satisfied [27]. It is not difficult to see from the perturbation series in Eq. (7) that $-\chi$ coincides with the zero-frequency Fourier component of the on-site Green's function for bosons at $T = 0$,

$$i\mathcal{G}(t - t') = \langle \hat{T} \hat{a}_i(t) \hat{a}_i^\dagger(t') \rangle. \quad (9)$$

In Eq. (9), $\hat{a}_i(t)$ are Heisenberg operators and the angular brackets mean that the average is performed over the ground state of the system involving the bosons and bath.

To proceed, we single out the local part of the Hamiltonian $\hat{H}_l = \hat{H}_0 + \hat{H}_{bath} + \hat{H}_{coup}$ in Eqs. (2)-(4), and employ the well-known Lang-Firsov transformation to obtain the new local Hamiltonian

$$\hat{H}_l' = \hat{S} \hat{H}_l \hat{S}^{-1}, \quad \hat{S} = \exp \left\{ \sum_{i\alpha} \frac{g_\alpha}{\varepsilon_\alpha} \hat{n}_i (\hat{b}_{i\alpha}^\dagger - \hat{b}_{i\alpha}) \right\}. \quad (10)$$

After standard manipulations [28], we obtain

$$\hat{H}_l' = \sum_i \frac{U'}{2} \hat{n}_i (\hat{n}_i - 1) - \mu' \sum_i \hat{n}_i + \sum_{i\alpha} \varepsilon_\alpha \hat{b}_{i\alpha}^\dagger \hat{b}_{i\alpha}, \quad (11)$$

where

$$U' = U - 2 \sum_\alpha \frac{g_\alpha^2}{\varepsilon_\alpha}, \quad \mu' = \mu + \sum_\alpha \frac{g_\alpha^2}{\varepsilon_\alpha}. \quad (12)$$

We assume weak coupling to the bath which implies that U' is positive. The transformation Eq. (10) means that the Green's function Eq. (9) can be re-expressed in terms of the operators $\hat{a}_i' = \hat{S} \hat{a}_i \hat{S}^{-1}$, defined in the Heisenberg representation with respect to \hat{H}_l' . Subsequent calculations are tedious but similar to those considered in Ref. [29]. Hence,

$$i\mathcal{G}(t - t') = i\mathcal{G}_0(t - t') F(t - t'), \quad (13)$$

with

$$F(t - t') = \exp \left\{ - \sum_\alpha (g_\alpha / \varepsilon_\alpha)^2 \left(1 - e^{-i\varepsilon_\alpha |t - t'|} \right) \right\}, \quad (14)$$

and

$$\begin{aligned} i\mathcal{G}_0(t - t') = & (n_0 + 1) e^{i|\xi - |(t' - t)|} \theta(t - t') \\ & + n_0 e^{i\xi_+(t - t')} \theta(t' - t), \end{aligned} \quad (15)$$

where ξ_{\pm} are the energies of particle-hole excitations

$$\xi_+ = \mu' - U'(n_0 - 1) > 0, \quad \xi_- = \mu' - U'n_0 < 0. \quad (16)$$

At $T = 0$, the ground state occupation for bosons in Mott-insulating phases is determined as $n_0 = n_0(\mu'/U') = \text{Integer}[\mu'/U'] + 1$, or $n_0 = 0$, if $\mu' < 0$, where U' and μ' are defined in Eq. (12). Using Eq. (5), one can easily show that $(\sum_{\alpha} \rightarrow \int_0^{\infty} d\varepsilon)$

$$F(t - t') = (1 + i\Lambda|t - t'|)^{-\eta}, \quad (17)$$

so that the equation for the phase boundary separating the insulating and superfluid phases is recast as

$$\begin{aligned} \frac{1}{zJ} &= -i\mathcal{G}(\omega = 0) \\ &= \int_0^{\infty} \frac{dx}{(1 + x\Lambda)^{\eta}} \left[(n_0 + 1)e^{-x|\xi_-|} + n_0 e^{-x\xi_+} \right], \end{aligned} \quad (18)$$

where x is an auxiliary variable of integration. The integral in Eq. (18) can be further expressed as a linear combination of confluent hypergeometric functions, albeit we have found it more convenient to integrate numerically to obtain the $T = 0$ phase diagram.

The form of the coupling in Eq. (5) implies that $U' = U - 2\eta\Lambda$ and $\mu' = \mu + \eta\Lambda$. This leads to two new important parameters η and $\eta\Lambda/U$ in the problem as a result of coupling to a bath. We only consider the situation in which $\eta\Lambda/U \ll 1$, so that the suppression of the bare interaction U is not too strong. This means that η can be comparable to unity only if $\Lambda/U \ll 1$. Such a case corresponds physically to a narrow band of low-energy bath degrees of freedom strongly interacting with the lattice bosons, and is different from the picture in which $\Lambda \sim O(U)$ but the coupling is weak, $\eta \ll 1$. The first scenario is close in spirit to the model considered in Ref. [24], although in both cases novel features appear on the mean-field phase diagram.

Figures 1 and 2 display mean field phase diagrams calculated from Eq. (18) in the limits of $\Lambda/U > 1$ and $\Lambda/U \ll 1$ respectively, for several values of η , such that $\eta\Lambda/U < 0.25$ in all cases. Since n_0 is determined by μ' and U' , a given occupation number corresponds to lower μ/U in comparison to the case in which $\eta = 0$.

An important feature to note is the difference in the functional behavior of the phase boundary near the points of integer μ'/U' for a) weak bath coupling, $\eta < 1$; and b) strong bath coupling, $\eta > 1$. From Eq. (18) it follows that for $\eta > 1$, the integral over x converges even if we put ξ_+ or ξ_- equal to zero, in contrast with the case $\eta < 1$. We consider these two cases separately and find the corresponding behavior close to the degeneracy points. If one moves along the upper branch of the lobe corresponding to the occupation number n_0 towards the point $(\mu'/U') = n_0$ from below, $|\xi_-| \rightarrow 0$ and

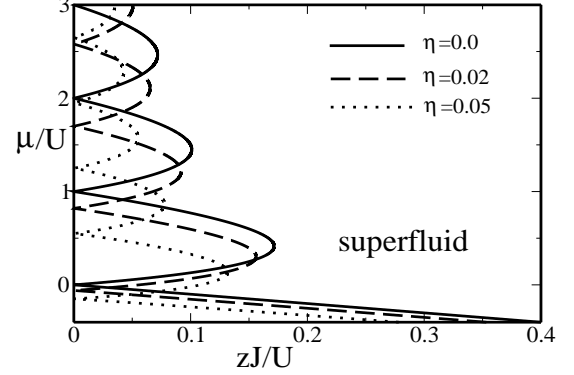


FIG. 1: Phase diagrams in the zJ/U - μ/U plane for $\Lambda/U = 3.0$, and $\eta = 0.0, 0.02$, and 0.05 . The internal parts of all lobes correspond to Mott phases with occupation number $n_0 = \text{Integer}[\mu'/U'] + 1$.

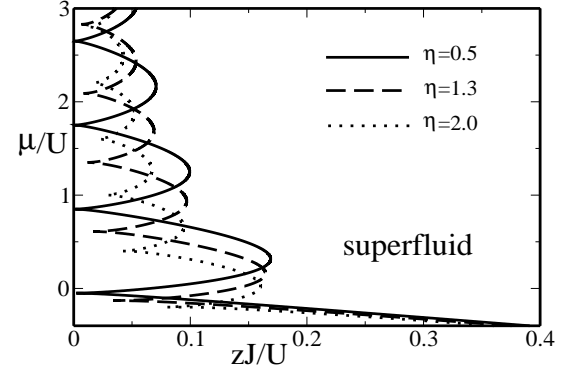


FIG. 2: Phase diagrams for $\Lambda/U = 0.1$ and $\eta = 0.5, 1.3$, and 2.0 . The meaning of regions is as in the previous figure. For $\eta = 1.3$ and 2.0 , the horizontal lines between $zJ = 0$ and zJ_- separating the Mott regions with n_0 differing by one are not shown.

$\xi_+ \rightarrow U$. At the same time, approaching the same point from above following the lower branch of the $n_0 + 1$ lobe, $|\xi_-| \rightarrow U$ whilst $\xi_+ \rightarrow 0$. Hence: a) If $\eta < 1$, it is easy to find the corresponding asymptotics for zJ from Eq. (18) for small $|\xi_-|$ or ξ_+ : close to the point $(\mu'/U') = n_0$, $zJ \propto |\xi_-|^{1-\eta}$ for the lower branch, and $zJ \propto \xi_+^{1-\eta}$ for the upper one. This behavior suggests a slightly narrower region of superfluid phase between the adjacent Mott lobes than would occur for $\eta = 0$. b) For $\eta > 1$, there is never a superfluid at $zJ = 0$ and a finite value of zJ is required to achieve superfluidity for any value of the chemical potential μ . Denoting as zJ_- and zJ_+ the limits obtained exactly at $(\mu'/U') = n_0$ for the lower and

upper branches respectively, we find from Eq. (18), that

$$\frac{1}{zJ_{\pm}} = \int_0^{\infty} \frac{dx}{(1+x\Lambda)^{\eta}} [(n_0+1) + (n_0+1 \pm 1)e^{-xU}],$$

These two limiting values are not equal to each other: $zJ_+ > zJ_-$, and for $\Lambda/U \ll 1$ differ from each other by $O(\Lambda^2/U^2)$. At the lowest order in Λ/U , $zJ_{\pm} \approx (n_0+1)(\eta-1)(\Lambda/U)$. The horizontal line between zJ_+ and zJ_- , albeit short, separates the superfluid phase from the Mott insulator having occupation number equal to n_0 . There is also a line between $zJ = 0$ and zJ_- (not shown in Fig. 2) which separates Mott states with occupation n_0 and n_0+1 . These two features of the mean-field diagram are new and arise as a result of strong interaction between the bosons and bath.

It should be emphasised that whilst our results are mean field expressions for the BHM coupled to a bath at zero temperature, they form the basis for further investigations of effects beyond mean field theory and at finite temperatures. We expect that the addition of fluctuations beyond mean field theory will modify our expressions for the phase boundary between Mott insulating and superfluid phases, although the result that a finite value of J is required for superfluidity at all μ will be robust. At low, but finite temperatures, there will be depletion of the condensate and, as a consequence, enlargement of non-superfluid parts of the phase diagram. Studies of the BHM (in the absence of a bath) indicate that the changes from the $T = 0$ case are largest around the points where μ/U is an integer [13]. Hence, in analogy with Ref. [13] we expect that, for $\eta < 1$, superfluidity will be suppressed around the points $(\mu'/U') = n_0$. For $\eta > 1$, in its turn, the transition between n_0 and n_0+1 Mott states at small J becomes a crossover, while the superfluid regions on the whole will be shifted towards larger zJ/U .

In addition to the general features we have outlined above, it is also of interest to connect our results to experiments in optical lattices. These experiments are performed in the presence of confining magnetic traps, rather than the uniform system considered above. This means that the trap potential $-V(\mathbf{r})$ must be added to the chemical potential μ . This leads to the appearance of the so-called “wedding cake” structure [25, 30] consisting of concentric regions of Mott phases separated by shells of superfluidity in which atoms are mobile. Our results indicate that coupling to the bath decreases the thickness of the shells, thus facilitating the crossover from superfluid to insulator upon increasing U/J .

It should be emphasized that the model discussed here is independent of other mechanisms of dissipation, such as excitation of the phase slips in a moving condensate observed recently [20, 21]. If a heat bath plays a role in experiments on cold atoms in optical lattices, then it would be highly desirable to have a way to determine its

strength. Unfortunately, however, for the model considered here, it is difficult to determine from the currently available experimental data how strong interaction with the bath may be. However, we believe that this particle-conserving interaction is not unrealistic on timescales relevant to experiments, and might be detected by performing lattice depth modulation experiments similar to those discussed in Ref. [31]. In these experiments, the lattice potential is modulated at a fixed frequency for a short period of time. The modulation effectively translates into variation of J . During this process, energy is transferred to the atoms resulting in heating and the broadening of the central momentum peak, indicating an increase in the non-superfluid fraction of the atoms as observed after ballistic expansion once the trap is switched off. The presence of coupling to a bath may mean that a system heated quickly by modulation will cool with time. Hence, varying the time between the end of the modulation and the free expansion may reveal a decrease of the out-of-condensate portion as a result of relaxation towards the initial equilibrium state giving a window to access the bath coupling.

In conclusion, we have performed an analysis of the effects of coupling the BHM to an ohmic bath on the mean field phase diagram of the BHM. We find that the changes from the absence of a bath depend on both the strength of the coupling to the bath and the width of the bath spectrum. We believe our work should be relevant to any physical system that can be modelled with a BHM.

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